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3-(4-N,N-dimethylaminophenyl)-2-nitro-1-phen-lprop-2-en-1-one by ^{13}C NMR spectroscopy and X-ray diffraction analysis

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Abstract

© 2016, Pleiades Publishing, Ltd.X-ray diffraction analysis established that 3-(4-N-N-dimethylaminophenyl)-2-nitro-1-phenylprop-2-en-1-one has E configuration both in crystal and in solution. The benzoyl group deviates from the styrene plane by 89.83°. The elongation of the C=C bond and shortening of its surrounding single bonds points to a high polarization of the molecule, implying a great contribution of the bipolar structure to the ground state.

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Keywords

13 C NMR spectroscopy, bipolar structure, X-ray diffraction analysis, zwitter ion, α-nitrochalcones